Supplementary Information (SI) for Inorganic Chemistry Frontiers.


# Fabrication of Multifunctional Ionic Covalent Organic Framework via Menshutkin Reaction and Ion-Exchange for Dual-Mode Detection of Organochlorine Pesticides and Design of Smartphone Sensing Platform

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## 1. Experimental section

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### 1.1. Materials

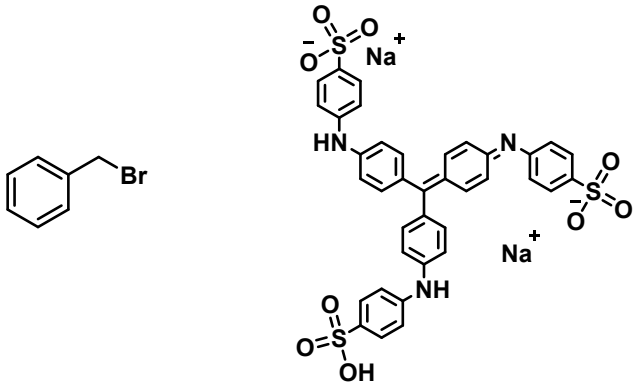
All the other solvents and reagents were obtained commercially and used without further purification. Deionized water was used throughout the experiments. 2,4,6-Tris(4-aminophenyl)triazine (Tta) (98%), tris(4-formylphenyl)amine (Tfa) (98%), benzyl bromide (BnBr) (98%), methyl blue (MB) (98%), 2,6-dichloro-4-nitroaniline (DCN) (95%), dicamba (DMA) (99%), agarose (AG) (95%), sulfamethoxazole (98%), flusilazole (98%), cyfluthrin (95%), carboxin (98%), alidochlor (97%), methylparaben (99%) and glyphosate (96%) were purchased from Adamas-beta. NaCl (99%), KCl (99%), $CaCl_2$ (96%), $MgCl_2$ (99%), $ZnCl_2$ (98%), $Na_2CO_3$ (99%), $Na_2SO_4$ (99%) were purchased from Sigma-Aldrich. Diethyl ether (98%) was purchased from Sinopharm. *n*-Butanol (*n*-BuOH) (99.5%), *o*-dichlorobenzene (*o*-DCB) (98%), acetic acid (AcOH) (99.8%), ethanol (EtOH) (95%), acetonitrile (MeCN) (99%), methanol (MeOH) (99.5%), tetrahydrofuran (THF) (99.5%), and N, N-dimethylformamide (DMF) (99.5%) were purchased from Greagent.

### 1.2. Instruments

The powder X-ray diffraction (PXRD) patterns were recorded on Bruker D8 ADVANCE diffractometer employing Cu Kα radiation (40 mA and 40 kV) with a 2θ range from 3° to 45° at room temperature. The surface morphology and EDS analysis were performed on Hitachi S-4800 field emission scanning electron microscope (SEM) with a voltage of 5 kV-15 kV. Fourier transform infrared (FT-IR) spectra were obtained by a Nexus 912 AO446 infrared spectrum radiometer in the wavenumber range of 4000 − 400 $cm^{-1}$. X-ray photoelectron spectroscopy (XPS) spectra were

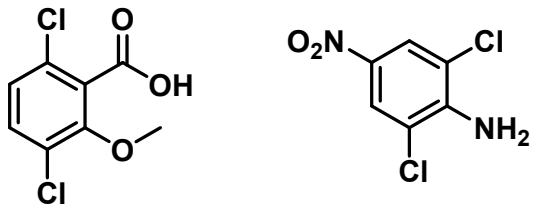
noted under the ultrahigh vacuum (< $10^{-6}$ Pa) at pass energy (93.90 eV) with Axis Ultra DLD spectrometer (Kratos, Japan) by employing an Mg Kα (1253.6 eV) anode. Thermogravimetric (TG) curves were measured on a TA TGA 55 system operating at a heating rate of 10 $^{o}$C/min in the range of 25 $^{o}$C up to 700 $^{o}$C under $N_2$ atmosphere. The fluorescence spectra were obtained on an Edinburgh FLS920 spectrophotometer employing 450 W xenon lamp as the source of excitation with appropriate cutoff filter. The UV-vis absorption spectra were carried on an Agilent 8453 spectrometer. The pH values of aqueous solutions were determined by an INESA PHS-25 pH meter with an E-201F pH composite electrode, which was carefully calibrated by standard buffer solution before testing. The HOMO-LUMO orbital energies were optimized by the B3LYP hybrid density functional and the basis set was 6-31G (d).

**Supporting figures**




**BnBr** **MB**

**Scheme S1** Structure of BnBr and MB.




**DMA** **DCN**

**Scheme S2** Structure of DMA and DCN.

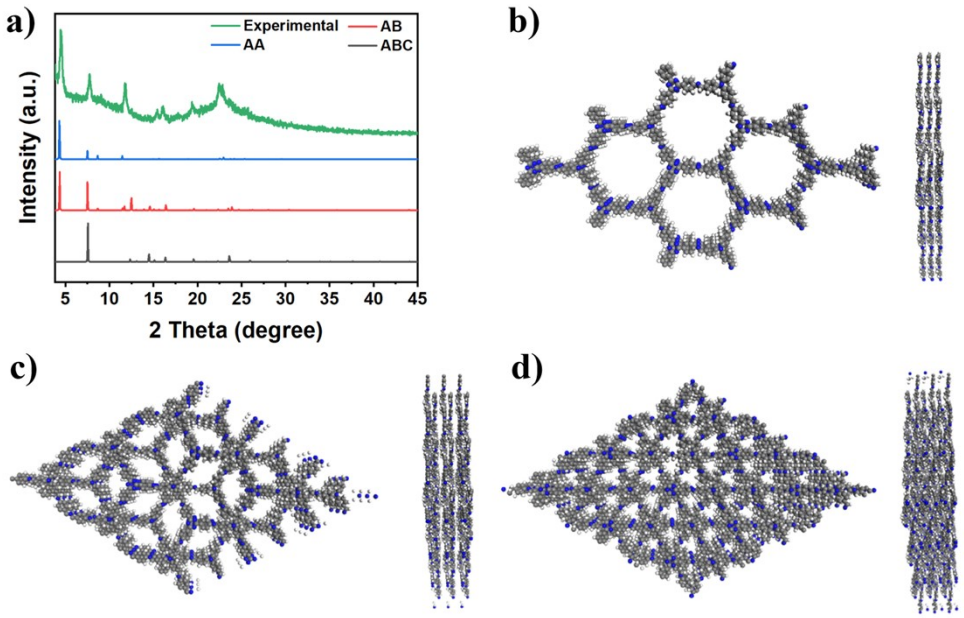



**Fig. S1** a) PXRD patterns of synthesized TfaTta and simulated TfaTta with AA, AB and ABC stacking modes. b) AA-stacking model, c) AB-stacking model and d) ABC-stacking model of TfaTta.

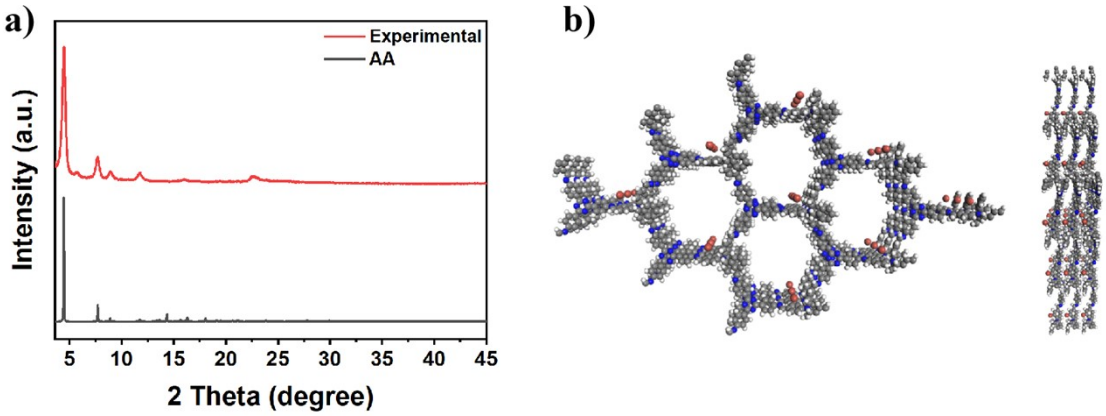



**Fig. S2** a) PXRD patterns of synthesized TfaTta-Br and simulated AA stacking mode of TfaTta-Br. b) AA-stacking model of TfaTta-Br.

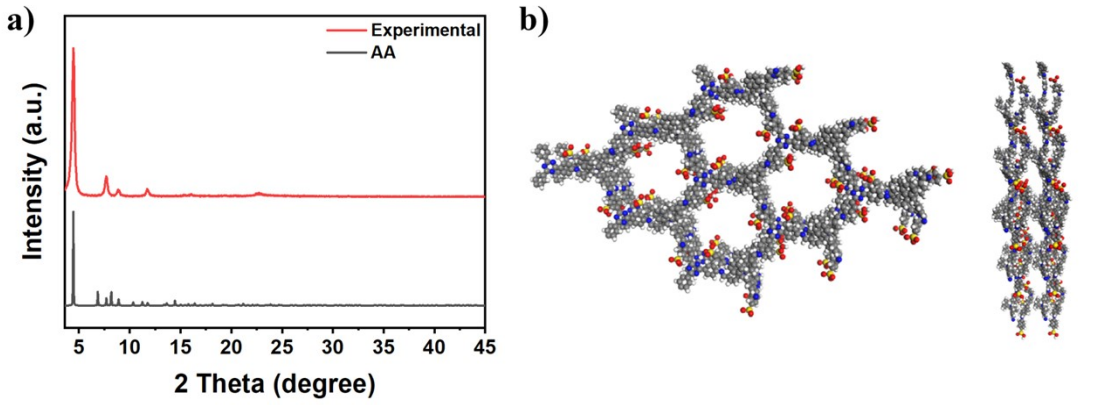



**Fig. S3** a) PXRD patterns of synthesized TfaTta-MB and simulated AA stacking mode of TfaTta-MB. b) AA-stacking model of TfaTta-MB.

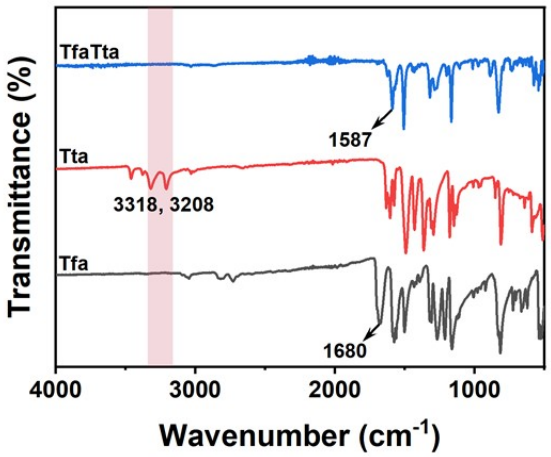



**Fig. S4** FT-IR spectra of Tfa, Tta and TfaTta.

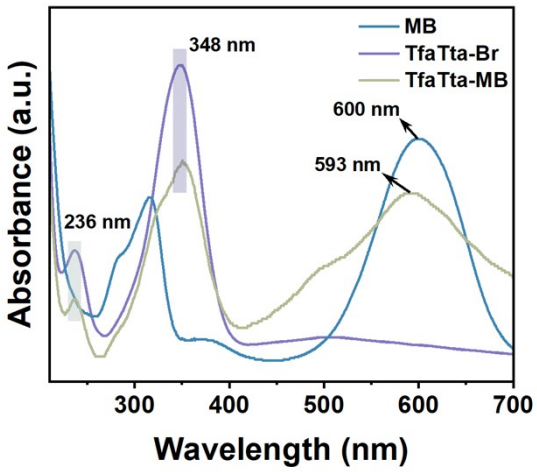



**Fig. S5** UV-vis absorption spectra of MB, TfaTta-Br and TfaTta-MB.

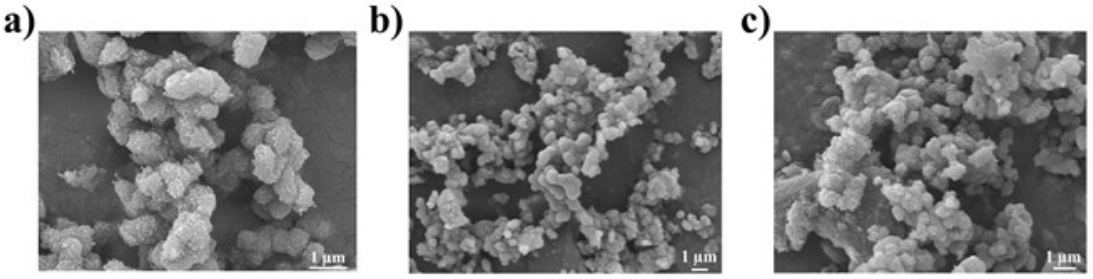
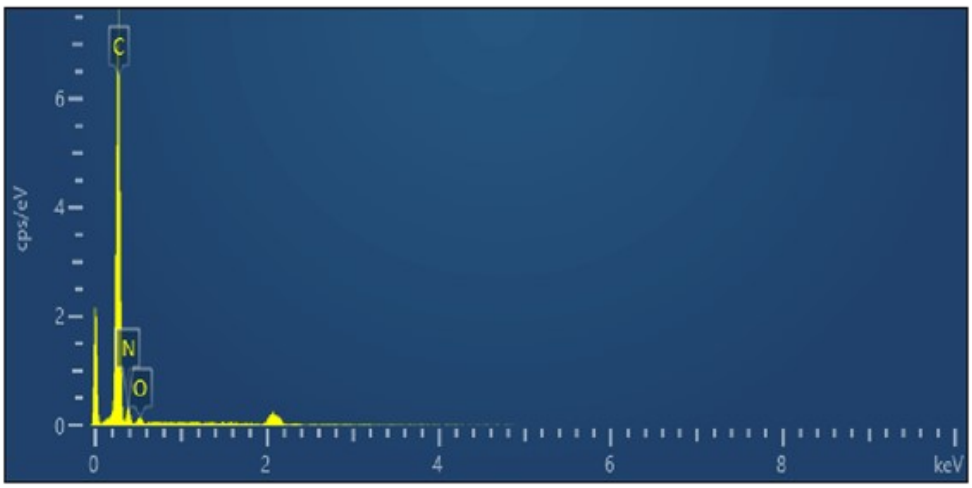
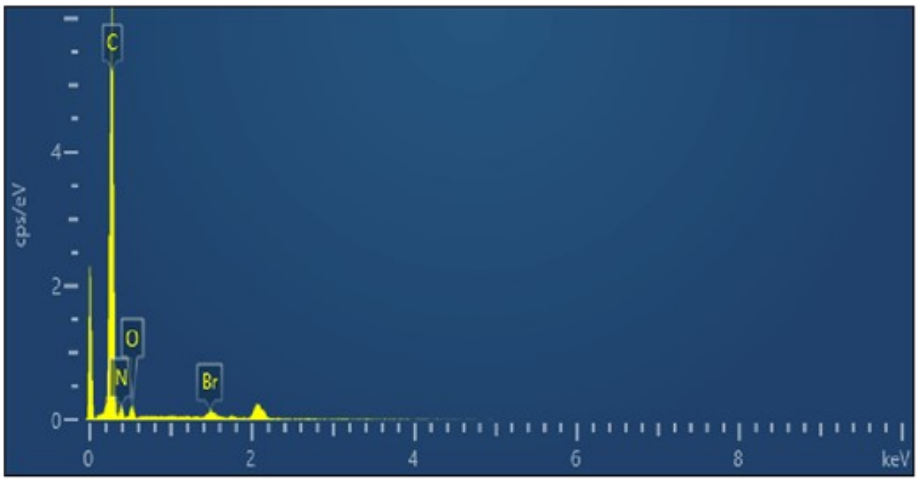



**Fig. S6** SEM image of a) TfaTta, b) TfaTta-Br and c) TfaTta-MB.



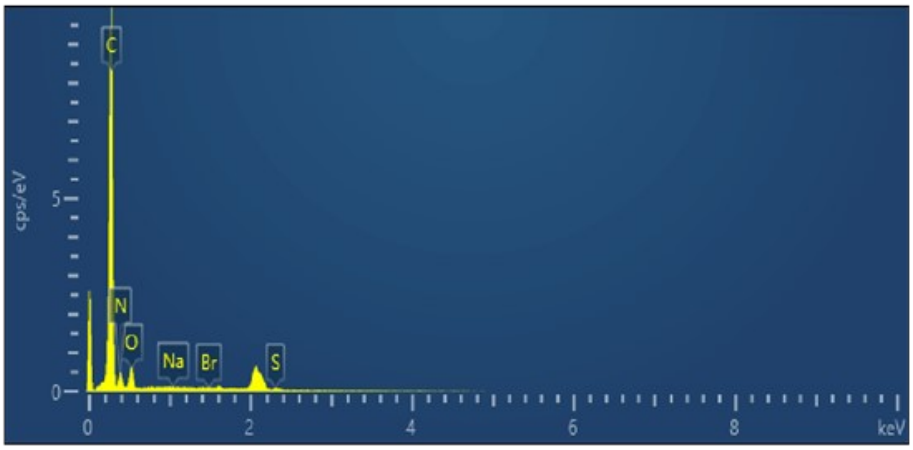

| Element | Wt % | Wt % Sigma |
|---|---|---|
| C | 85.25 | 1.13 |
| N | 12.65 | 1.10 |
| O | 2.10 | 0.39 |

**Fig. S7** EDS analysis of TfaTta.




| Element | Wt % | Wt % Sigma |
|---|---|---|
| C | 83.07 | 1.19 |
| N | 8.46 | 0.93 |
| O | 3.75 | 0.39 |
| Br | 4.71 | 0.86 |

**Fig. S8** EDS analysis of TfaTta-Br.




| Element | Wt % | Wt % Sigma |
|---|---|---|
| C | 79.01 | 0.85 |
| N | 10.85 | 0.73 |
| O | 6.80 | 0.35 |
| S | 3.34 | 0.54 |
| Br | 0.00 | 0.51 |
| Na | 0.00 | 0.16 |

**Fig. S9** EDS analysis of TfaTta-MB.

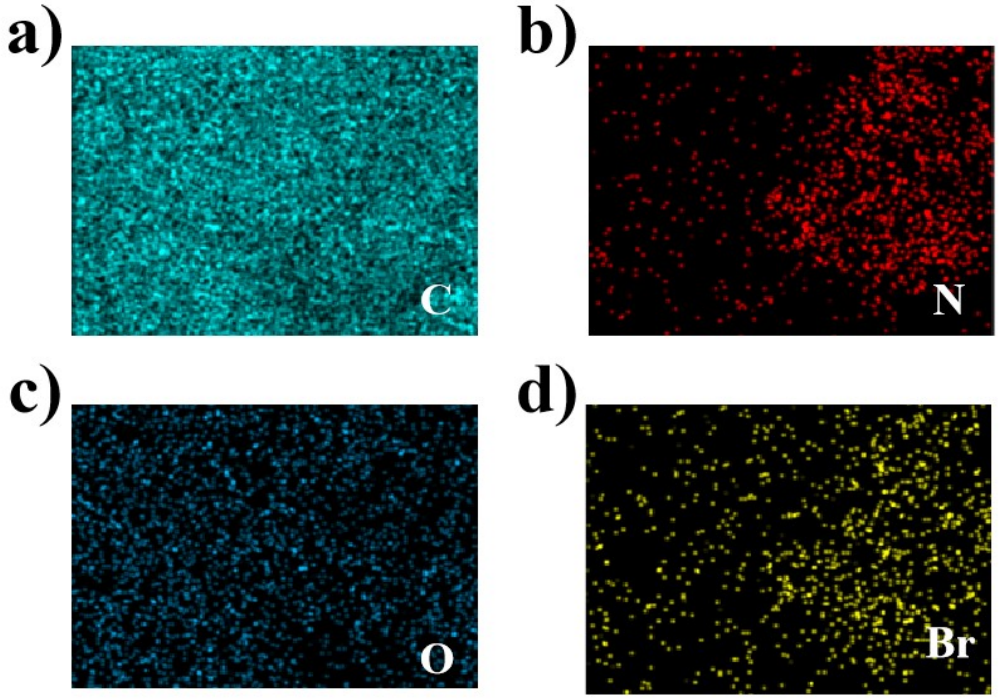



**Fig. S10** EDS mapping images of C, N, O and Br in TfaTta-Br.

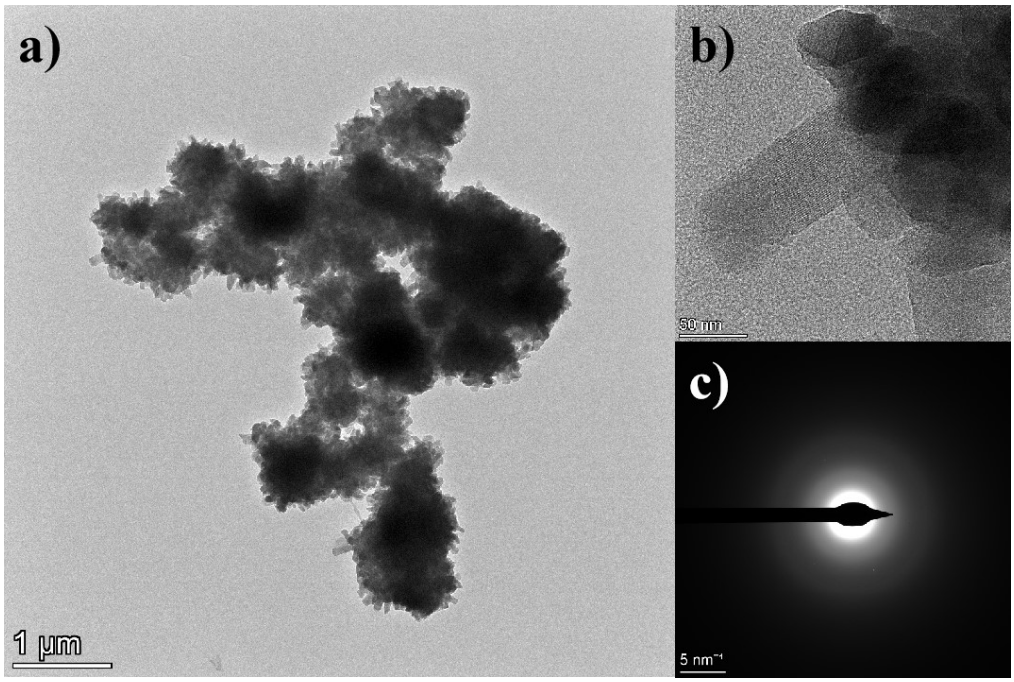



**Fig. S11** a-b) TEM image images and c) SAED pattern of TfaTta.

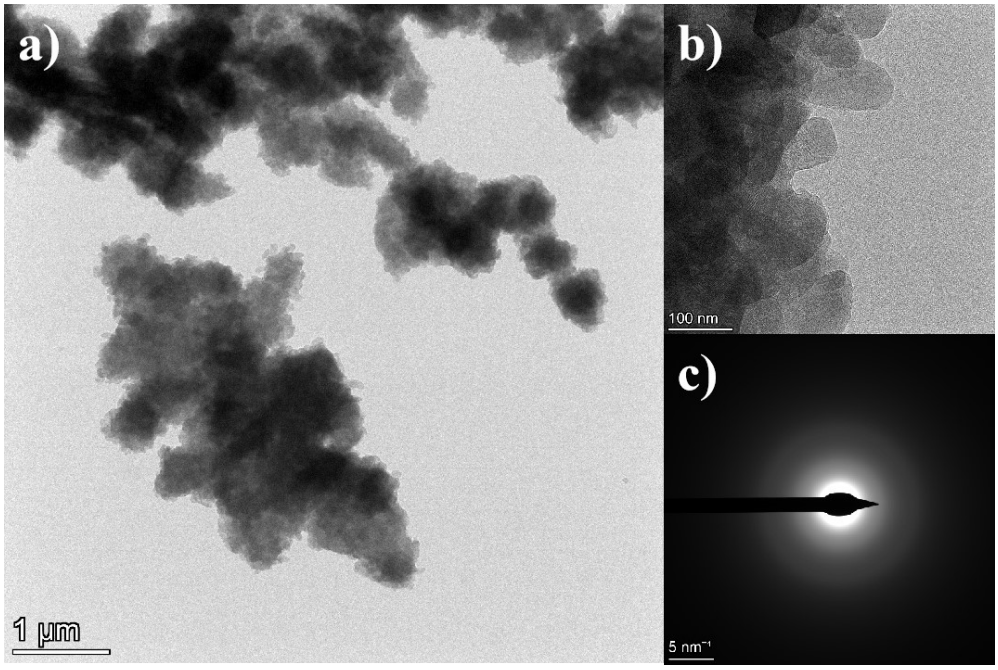



**Fig. S12** a-b) TEM image images and c) SAED pattern of TfaTta-Br.

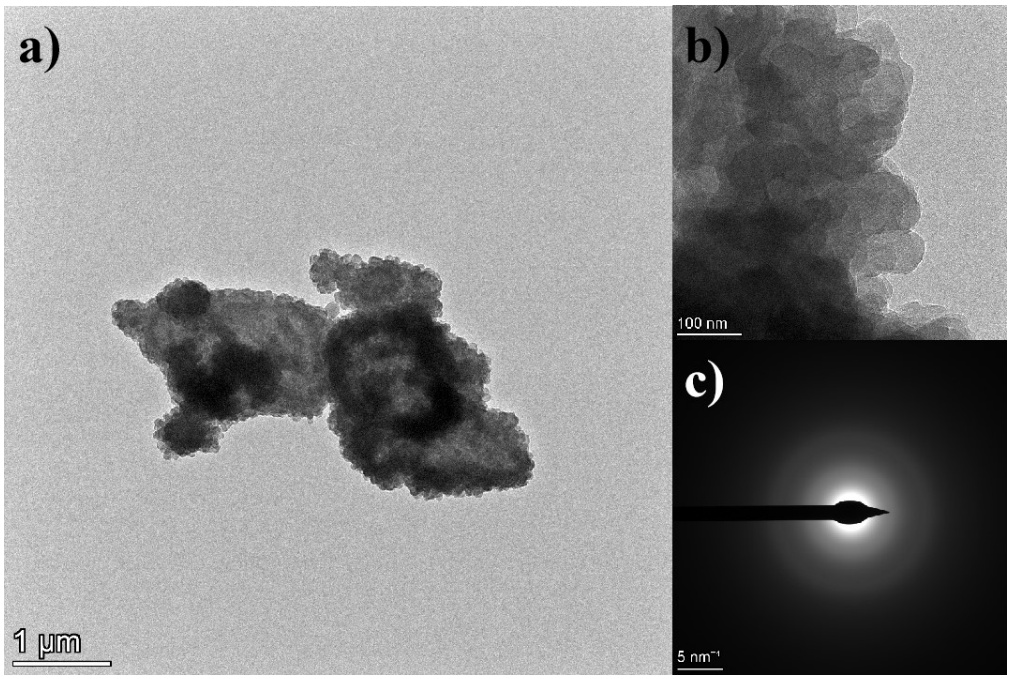



**Fig. S13** a-b) TEM images and c) SAED pattern of TfaTta-MB.

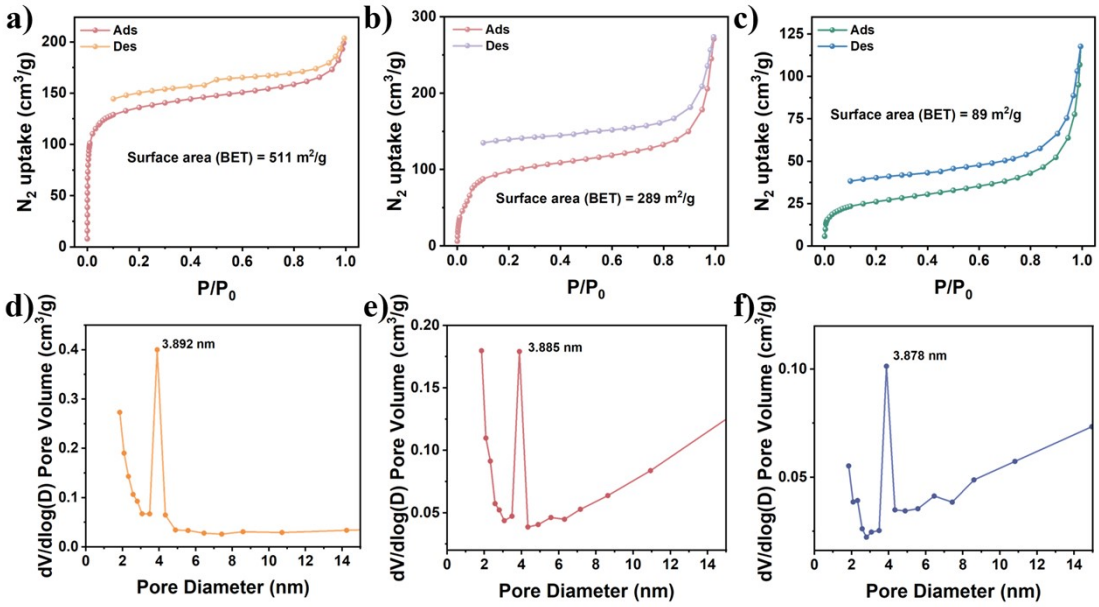



**Fig. S14** a-c) $N_2$ adsorption–desorption isotherms of TfaTta, TfaTta-Br and TfaTta-MB. d-f) Pore size distribution of TfaTta, TfaTta-Br and TfaTta-MB.

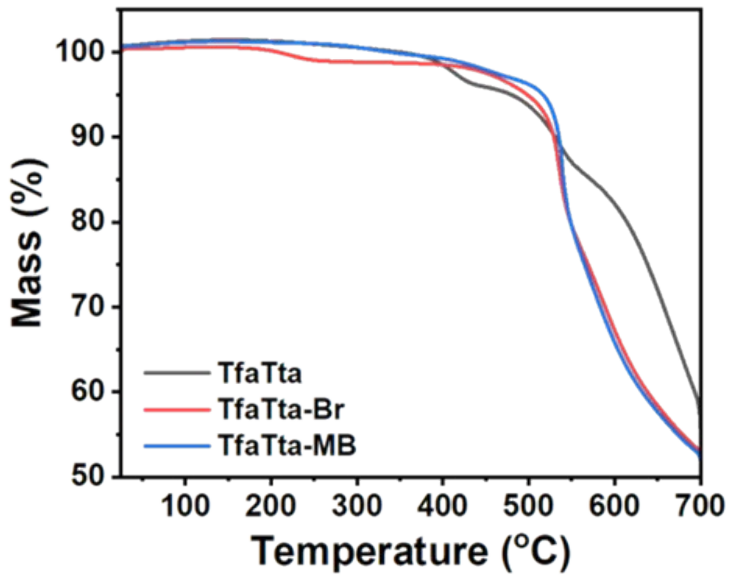



**Fig. S15** TGA analysis of TfaTta, TfaTta-Br and TfaTta-MB.

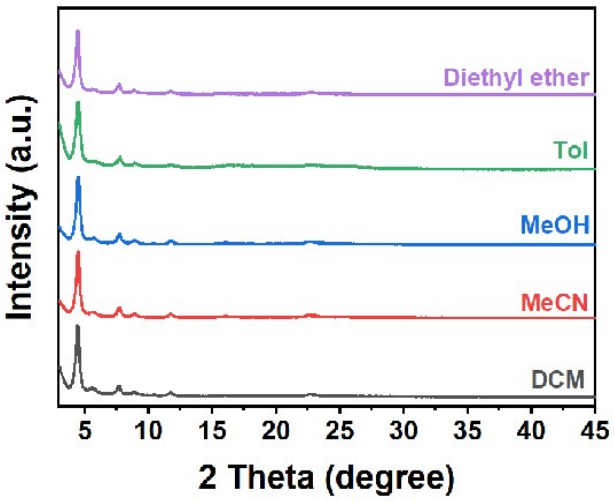



**Fig. S16** PXRD patterns of TfaTta-MB after soaking in different organic solvents for 48 h.

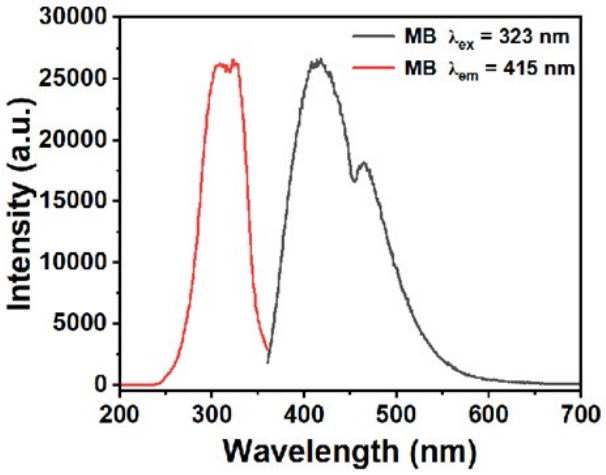



**Fig S17** Excitation and emission spectra of MB.

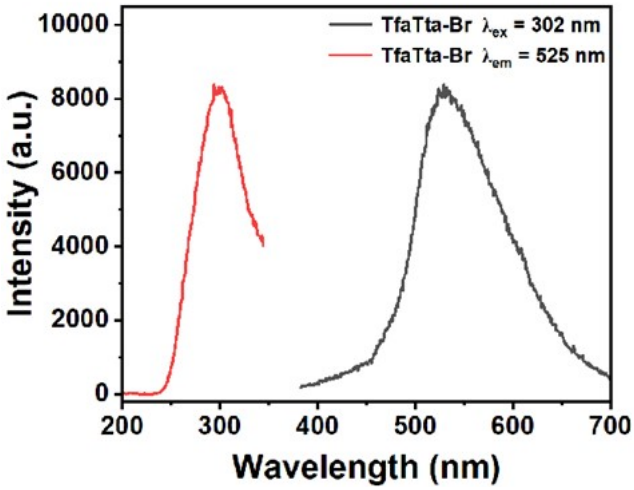



**Fig. S18** Excitation and emission spectra of TfaTta-Br.

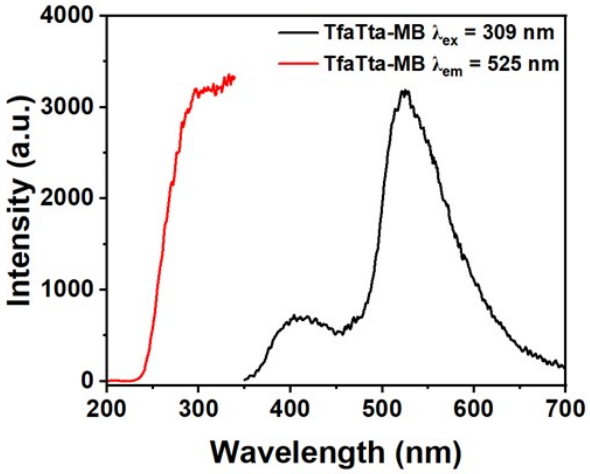



**Fig. S19** Excitation and emission spectra of TfaTta-MB.

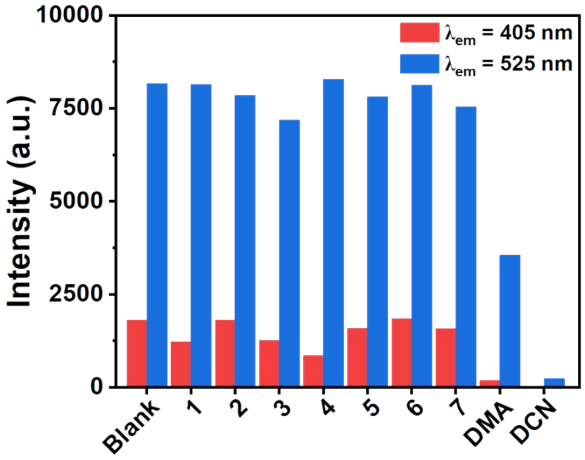



**Fig. S20** Selectivity ability of TfaTta-MB toward various pesticides (1. sulfamethoxazole; 2. flusilazole; 3. cyfluthrin; 4. carboxin; 5. alidochlor; 6. methylparaben; 7. glyphosate).

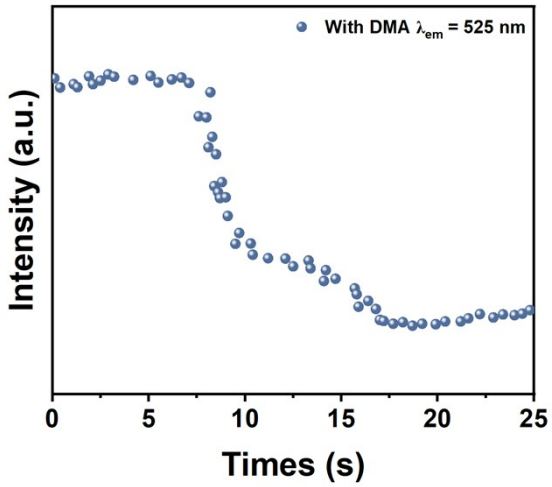



**Fig. S21** Response time of TfaTta-MB to DMA at the emission of 525 nm.

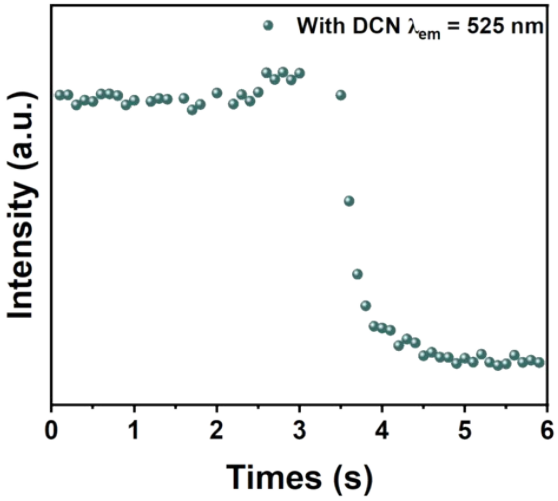



**Fig. S22** Response time of TfaTta-MB to DCN at the emission of 525 nm.

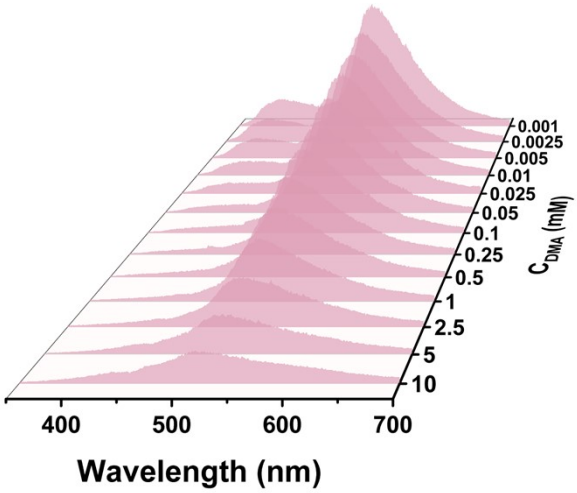



**Fig. S23** The emission spectra of TfaTta-MB upon the gradual addition of DMA.


**Fig. S24** The solvent of TfaTta-MB with and without DMA.

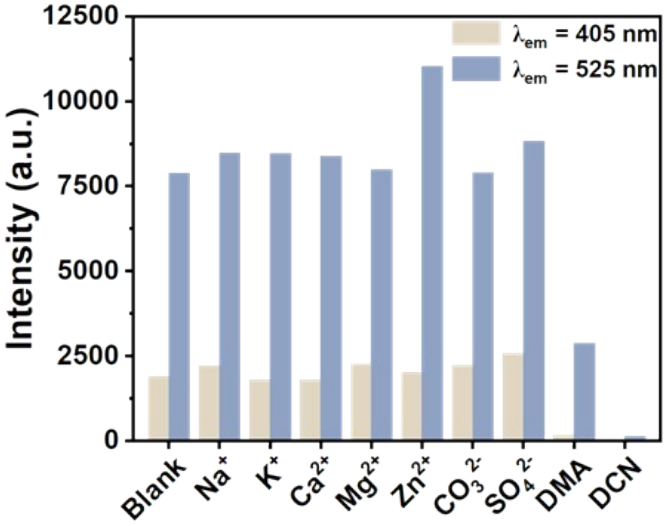



**Fig. S25** Selectivity ability of TfaTta-MB toward common ions.

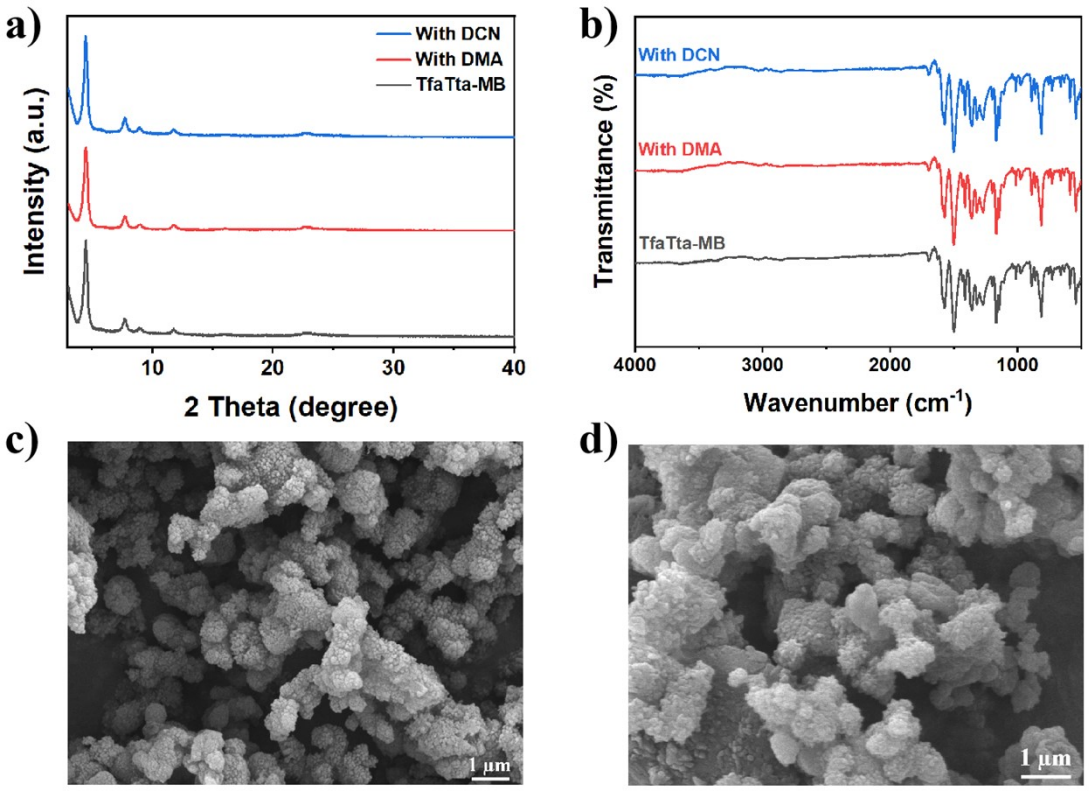



**Fig. S26** a) PXRD patterns, b) FT-IR spectra and c-d) SEM images of post-sensing materials.

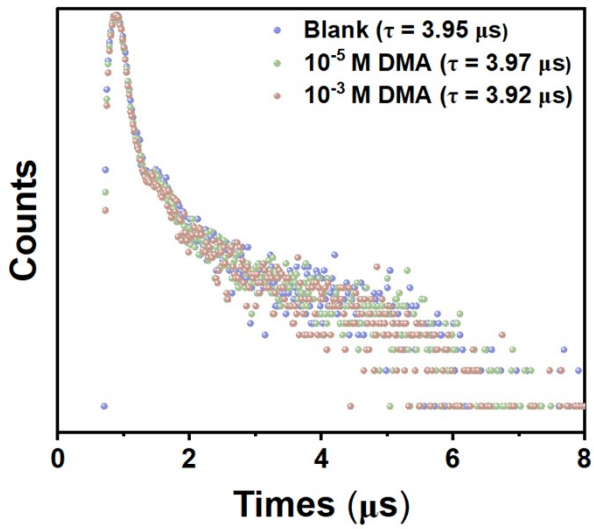



**Fig. S27** Lifetime decay curve ($\lambda_{ex}$ = 309 nm, $\lambda_{em}$ = 405 nm) of TfaTta-MB with and without DMA.

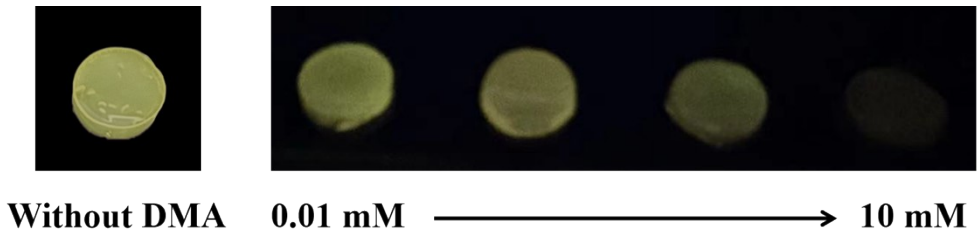



**Fig. S28** Photos of TfaTta-MB/AG under 365 nm UV light after immersing in different concentrations of DMA.

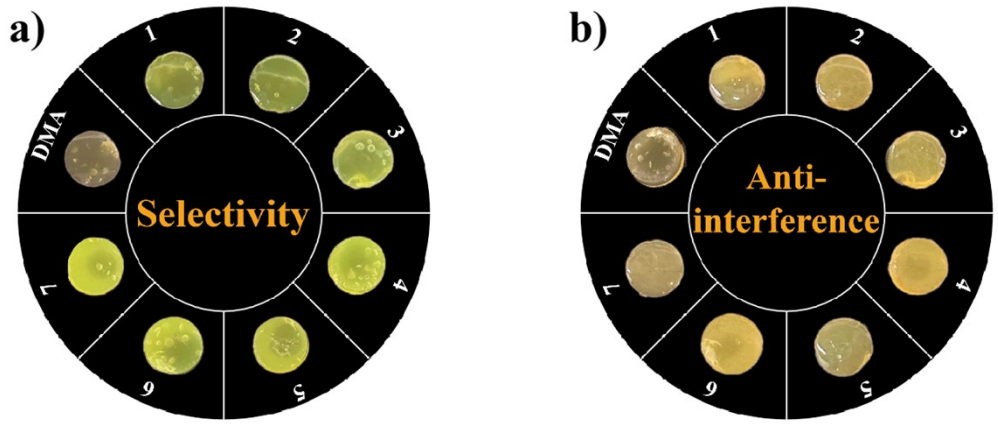



**Fig. S29** a) Selectivity and b) anti-interference ability of TfaTta-MB/AG towards different pesticides (1. sulfamethoxazole; 2. flusilazole; 3. cyfluthrin; 4. carboxin; 5. alidochlor; 6. methylparaben; 7. glyphosate).

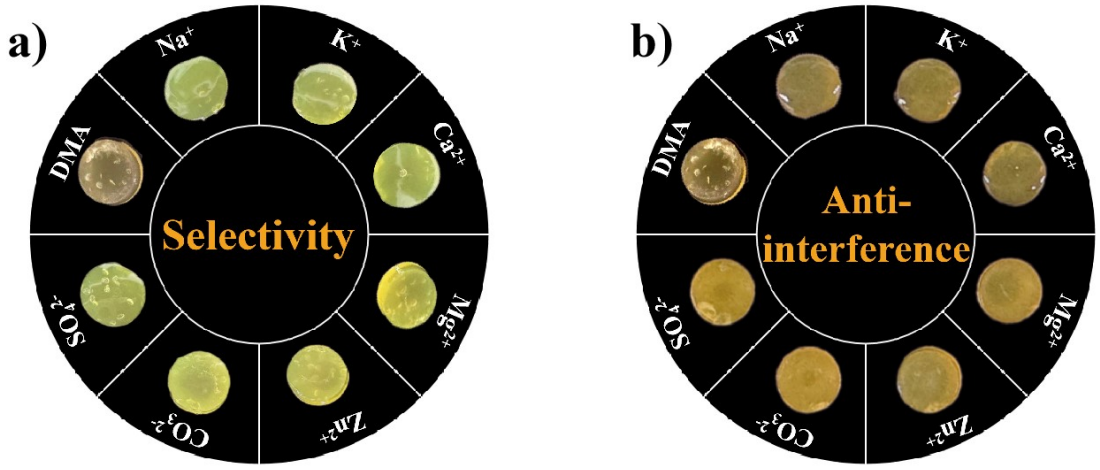



**Fig. S30** a) Selectivity and b) anti-interference ability of TfaTta-MB/AG towards different ions.

**Table S1** Fractional atomic coordinates of TfaTta.

| **Space group: P3**<br>***a* = 23.61 Å, *b* = 23.61 Å, *c* = 3.94 Å**<br>**α = β = 90°, γ = 120°** | | | |
|---|---|---|---|
| **Atom** | ***x* (Å)** | ***y* (Å)** | ***z* (Å)** |
| C1 | 0.73794 | 0.37633 | 0.08658 |
| C2 | 0.64258 | 0.42223 | -0.06951 |
| C3 | 0.60183 | 0.44933 | -0.06945 |
| C4 | 0.5402 | 0.41626 | 0.08549 |
| C5 | 0.52046 | 0.35598 | 0.24078 |
| C6 | 0.56159 | 0.32932 | 0.24217 |
| C7 | 0.49602 | 0.4436 | 0.08817 |
| N8 | 0.51301 | 0.49929 | -0.05678 |
| C9 | 0.47456 | 0.53094 | -0.07406 |
| C10 | 0.50608 | 0.59728 | -0.1604 |
| C11 | 0.47129 | 0.63075 | -0.17642 |
| C12 | 0.40375 | 0.59802 | -0.11052 |
| C13 | 0.37173 | 0.53097 | -0.03238 |
| C14 | 0.40666 | 0.49765 | -0.01439 |
| C15 | 0.36708 | 0.63374 | -0.11905 |
| N16 | 0.39953 | 0.70017 | -0.11874 |
| H17 | 0.68951 | 0.4499 | -0.18695 |
| H18 | 0.61867 | 0.49613 | -0.19179 |
| H19 | 0.47307 | 0.32936 | 0.36236 |
| H20 | 0.54367 | 0.28259 | 0.35996 |
| H21 | 0.44989 | 0.4169 | 0.22056 |
| H22 | 0.5581 | 0.62335 | -0.21193 |

| | | | |
|---|---|---|---|
| H23 | 0.49732 | 0.68221 | -0.24115 |
| H24 | 0.31968 | 0.50424 | 0.0182 |
| H25 | 0.38001 | 0.44597 | 0.04244 |
| N26 | 0.66667 | 0.33333 | 0.08684 |

**Table S2** Fractional atomic coordinates of TfaTta-Br.

| **Space group: P1**<br>***a* = 6.50 Å, *b* = 22.99 Å, *c* = 22.91 Å**<br>**α = 60°, β = γ = 90°** | | | |
|---|---|---|---|
| **Atom** | ***x* (Å)** | ***y* (Å)** | ***z* (Å)** |
| C1 | -1.11135 | 0.28272 | -0.93748 |
| C2 | -1.01718 | 0.15818 | -0.81579 |
| C3 | -0.98803 | 0.09025 | -0.76982 |
| C4 | -1.14867 | 0.05183 | -0.72744 |
| C5 | -1.33123 | 0.0839 | -0.72711 |
| C6 | -1.36124 | 0.1519 | -0.77403 |
| C7 | -1.12902 | -0.02157 | -0.68538 |
| N8 | -1.00506 | -0.05387 | -0.70374 |
| C9 | -0.97783 | -0.12533 | -0.6693 |
| C10 | -0.91308 | -0.1554 | -0.70634 |
| C11 | -0.88569 | -0.22497 | -0.67481 |
| C12 | -0.91776 | -0.26538 | -0.60514 |
| C13 | -0.97848 | -0.23484 | -0.56782 |
| C14 | -1.00904 | -0.16553 | -0.59956 |
| C15 | -0.88779 | -0.33894 | -0.5709 |
| N16 | -0.89417 | -0.37237 | -0.6058 |
| H17 | -0.88686 | 0.18583 | -0.84593 |
| H18 | -0.84029 | 0.06756 | -0.76794 |
| H19 | -1.45395 | 0.05583 | -0.6923 |
| H20 | -1.50475 | 0.17418 | -0.77164 |
| H21 | -1.23236 | -0.04845 | -0.64306 |
| H22 | -0.88629 | -0.12481 | -0.76003 |
| H23 | -0.83722 | -0.24699 | -0.70475 |
| H24 | -1.00399 | -0.26459 | -0.51399 |
| H25 | -1.05348 | -0.14352 | -0.56931 |
| C26 | -1.2129 | 0.18886 | -0.82476 |
| C27 | -1.03458 | 0.30394 | -0.82049 |
| C28 | -1.00522 | 0.34194 | -0.78889 |
| C29 | -1.16844 | 0.37853 | -0.78304 |
| C30 | -1.36098 | 0.37638 | -0.80917 |
| C31 | -1.39211 | 0.33786 | -0.84002 |
| C32 | -1.14212 | 0.41999 | -0.75087 |

| | | | |
|---|---|---|---|
| N33 | -0.98414 | 0.41242 | -0.71282 |
| C34 | -0.95063 | -0.54893 | -0.68003 |
| C35 | -0.84954 | -0.5789 | -0.61769 |
| C36 | -0.82271 | -0.54365 | -0.58303 |
| C37 | -0.89203 | -0.47696 | -0.61112 |
| C38 | -0.98562 | -0.44606 | -0.67505 |
| C39 | -1.01542 | -0.4817 | -0.70907 |
| C40 | -0.87328 | -0.4404 | -0.57329 |
| N41 | -0.84643 | -0.47482 | -0.50522 |
| H42 | -0.90364 | 0.27747 | -0.82492 |
| H43 | -0.85393 | 0.34334 | -0.76983 |
| H44 | -1.4893 | 0.40436 | -0.80524 |
| H45 | -1.54584 | 0.33868 | -0.85815 |
| H46 | -1.26372 | 0.45486 | -0.75683 |
| H47 | -0.79626 | -0.63033 | -0.5951 |
| H48 | -0.74826 | -0.56869 | -0.53418 |
| H49 | -1.03987 | -0.39468 | -0.69831 |
| H50 | -1.08809 | -0.4565 | -0.75817 |
| C51 | -1.22901 | 0.30033 | -0.84673 |
| C52 | -1.06946 | 0.35227 | -0.97941 |
| C53 | -0.98091 | 0.37728 | -1.04319 |
| C54 | -0.93614 | 0.33411 | -1.0682 |
| C55 | -0.97067 | 0.26541 | -1.02719 |
| C56 | -1.05379 | 0.24004 | -0.9631 |
| C57 | -0.87009 | 0.35952 | -1.13841 |
| N58 | -0.87441 | 0.42332 | -1.1819 |
| C59 | -0.8404 | -0.54615 | -0.25322 |
| C60 | -0.81695 | -0.47645 | -0.29025 |
| C61 | -0.80842 | -0.44292 | -0.36046 |
| C62 | -0.82473 | -0.47859 | -0.3954 |
| C63 | -0.8409 | -0.54891 | -0.35821 |
| C64 | -0.84974 | -0.58248 | -0.28778 |
| C65 | -0.83972 | -0.44173 | -0.46991 |
| N66 | -0.86129 | -0.37403 | -0.50323 |
| H67 | -1.11621 | 0.38844 | -0.96492 |
| H68 | -0.95718 | 0.43092 | -1.0742 |
| H69 | -0.94316 | 0.23128 | -1.04603 |
| H70 | -1.09278 | 0.18724 | -0.93662 |
| H71 | -0.83025 | 0.32339 | -1.15365 |
| H72 | -0.81114 | -0.44773 | -0.26454 |
| H73 | -0.79491 | -0.38871 | -0.38735 |
| H74 | -0.85471 | -0.57785 | -0.38352 |
| H75 | -0.87257 | -0.6362 | -0.26145 |

| | | | |
|---|---|---|---|
| N76 | -1.25361 | 0.25874 | -0.87913 |
| C77 | -1.46665 | 0.26505 | -0.90853 |
| C78 | -1.5011 | 0.22633 | -0.94577 |
| C79 | -1.48315 | 0.25967 | -1.01653 |
| C80 | -1.50219 | 0.22417 | -1.05107 |
| C81 | -1.54747 | 0.15563 | -1.01582 |
| C82 | -1.57371 | 0.12254 | -0.94601 |
| C83 | -1.5508 | 0.15756 | -0.91111 |
| H84 | -1.49903 | 0.31895 | -0.94506 |
| H85 | -1.58937 | 0.25035 | -0.87035 |
| H86 | -1.44817 | 0.31283 | -1.04477 |
| H87 | -1.48352 | 0.24998 | -1.10524 |
| H88 | -1.56403 | 0.1283 | -1.04266 |
| H89 | -1.61133 | 0.06957 | -0.91881 |
| H90 | -1.57316 | 0.13073 | -0.85732 |
| Br91 | -0.60692 | 0.21013 | -1.66113 |

**Table S3** Fractional atomic coordinates of TfaTta-MB.

| **Space group: P1**<br>***a* = 23.01 Å, *b* = 22.88 Å, *c* = 12.88 Å**<br>**α =β =90°, γ = 120°** | | | |
|---|---|---|---|
| **Atom** | ***x* (Å)** | ***y* (Å)** | ***z* (Å)** |
| C1 | 0.73582 | 0.37353 | 1.70175 |
| C2 | 0.63179 | 0.3808 | 1.57992 |
| C3 | 0.58779 | 0.39975 | 1.53685 |
| C4 | 0.52474 | 0.37739 | 1.58179 |
| C5 | 0.50384 | 0.33095 | 1.66313 |
| C6 | 0.54843 | 0.31374 | 1.70784 |
| C7 | 0.48203 | 0.40532 | 1.55094 |
| N8 | 0.50928 | 0.46945 | 1.53348 |
| C9 | 0.47411 | 0.50633 | 1.52314 |
| C10 | 0.50977 | 0.57589 | 1.54183 |
| C11 | 0.47705 | 0.61354 | 1.54132 |
| C12 | 0.40782 | 0.58204 | 1.52287 |
| C13 | 0.37229 | 0.51241 | 1.50116 |
| C14 | 0.40509 | 0.47484 | 1.50036 |
| C15 | 0.37207 | 0.62052 | 1.53339 |
| N16 | 0.40707 | 0.68899 | 1.54032 |
| H17 | 0.67802 | 0.39602 | 1.53848 |
| H18 | 0.60303 | 0.43199 | 1.4687 |
| H19 | 0.4538 | 0.31004 | 1.69522 |
| H20 | 0.52954 | 0.27736 | 1.77004 |
| H21 | 0.42847 | 0.37457 | 1.56342 |

| | | | |
|---|---|---|---|
| H22 | 0.56297 | 0.60084 | 1.55862 |
| H23 | 0.50592 | 0.66696 | 1.55839 |
| H24 | 0.3189 | 0.4869 | 1.48622 |
| H25 | 0.37614 | 0.42154 | 1.4826 |
| C26 | 0.61629 | 0.34448 | 1.67508 |
| C27 | 0.65004 | 0.24491 | 1.59637 |
| C28 | 0.62909 | 0.17931 | 1.56288 |
| C29 | 0.59746 | 0.12527 | 1.63188 |
| C30 | 0.58869 | 0.13801 | 1.73524 |
| C31 | 0.61125 | 0.20386 | 1.76964 |
| C32 | 0.57023 | 0.05572 | 1.59421 |
| N33 | 0.52202 | 0.00649 | 1.64553 |
| C34 | 0.48672 | 0.93625 | 1.61936 |
| C35 | 0.43063 | 0.89364 | 1.67899 |
| C36 | 0.39397 | 0.8248 | 1.6584 |
| C37 | 0.41313 | 0.79704 | 1.57758 |
| C38 | 0.46939 | 0.83932 | 1.51744 |
| C39 | 0.50611 | 0.90877 | 1.5381 |
| C40 | 0.3748 | 0.72392 | 1.55907 |
| N41 | 0.30718 | 0.69016 | 1.57116 |
| H42 | 0.67185 | 0.28546 | 1.54094 |
| H43 | 0.63653 | 0.17085 | 1.4825 |
| H44 | 0.56476 | 0.09699 | 1.79038 |
| H45 | 0.60245 | 0.20948 | 1.85004 |
| H46 | 0.588 | 0.04737 | 1.52132 |
| H47 | 0.41521 | 0.9143 | 1.74193 |
| H48 | 0.35096 | 0.79294 | 1.70629 |
| H49 | 0.48437 | 0.81881 | 1.4543 |
| H50 | 0.54925 | 0.93998 | 1.49044 |
| C51 | 0.64244 | 0.25935 | 1.70046 |
| C52 | 0.78198 | 0.34997 | 1.71315 |
| C53 | 0.85067 | 0.39219 | 1.69595 |
| C54 | 0.8762 | 0.45992 | 1.66869 |
| C55 | 0.83228 | 0.48521 | 1.66245 |
| C56 | 0.76387 | 0.44364 | 1.68224 |
| C57 | 0.9483 | 0.50517 | 1.64787 |
| N58 | 0.99049 | 0.48324 | 1.65569 |
| C59 | 0.061 | 0.52033 | 1.63252 |
| C60 | 0.09999 | 0.49152 | 1.66001 |
| C61 | 0.16825 | 0.52384 | 1.63554 |
| C62 | 0.19884 | 0.58596 | 1.5837 |
| C63 | 0.16002 | 0.61496 | 1.55547 |
| C64 | 0.09146 | 0.58202 | 1.57819 |

| | | | |
|---|---|---|---|
| C65 | 0.27159 | 0.62194 | 1.56368 |
| N66 | 0.30423 | 0.5873 | 1.54575 |
| H67 | 0.76507 | 0.29864 | 1.73743 |
| H68 | 0.88376 | 0.37209 | 1.7062 |
| H69 | 0.85103 | 0.53789 | 1.64479 |
| H70 | 0.73335 | 0.46742 | 1.68415 |
| H71 | 0.96481 | 0.55676 | 1.62556 |
| H72 | 0.07746 | 0.44378 | 1.70061 |
| H73 | 0.19768 | 0.50126 | 1.65958 |
| H74 | 0.18276 | 0.66297 | 1.51496 |
| H75 | 0.0632 | 0.60535 | 1.55245 |
| N76 | 0.66408 | 0.32973 | 1.73039 |
| C77 | 0.66108 | 0.3381 | 1.84612 |
| C78 | 0.68922 | 0.41063 | 1.88283 |
| C79 | 0.75303 | 0.44507 | 1.92889 |
| C80 | 0.78162 | 0.51328 | 1.95569 |
| C81 | 0.7468 | 0.54772 | 1.9359 |
| C82 | 0.68286 | 0.51352 | 1.89227 |
| C83 | 0.65358 | 0.44511 | 1.86728 |
| H84 | 0.68992 | 0.3175 | 1.88594 |
| H85 | 0.60965 | 0.30842 | 1.87807 |
| H86 | 0.78124 | 0.41946 | 1.94254 |
| H87 | 0.83126 | 0.53954 | 1.98976 |
| H88 | 0.76941 | 0.60076 | 1.95449 |
| H89 | 0.65606 | 0.54001 | 1.87558 |
| H90 | 0.6037 | 0.41986 | 1.83517 |
| C91 | 0.58388 | 1.109 | -0.77176 |
| C92 | 0.65179 | 1.14919 | -0.7988 |
| C93 | 0.68125 | 1.21929 | -0.80525 |
| C94 | 0.64391 | 1.25129 | -0.78423 |
| C95 | 0.57558 | 1.21076 | -0.75774 |
| C96 | 0.54556 | 1.14043 | -0.75463 |
| C97 | 0.67762 | 1.32675 | -0.78041 |
| C98 | 0.6461 | 1.36061 | -0.81161 |
| C99 | 0.74703 | 1.36423 | -0.73753 |
| C100 | 0.79761 | 1.42003 | -0.79072 |
| C101 | 0.8629 | 1.45484 | -0.75108 |
| C102 | 0.87861 | 1.43542 | -0.65732 |
| C103 | 0.82817 | 1.37968 | -0.604 |
| C104 | 0.76342 | 1.34343 | -0.64529 |
| C105 | 0.66624 | 1.42893 | -0.76952 |
| C106 | 0.63407 | 1.46145 | -0.79756 |
| C107 | 0.57955 | 1.43185 | -0.87588 |

| | | | |
|---|---|---|---|
| C108 | 0.56051 | 1.36526 | -0.92042 |
| C109 | 0.59068 | 1.33131 | -0.88933 |
| N110 | 0.54941 | 1.46349 | -0.90929 |
| C111 | 0.56009 | 1.52702 | -0.87139 |
| C112 | 0.53508 | 1.53108 | -0.77399 |
| C113 | 0.54301 | 1.59241 | -0.73896 |
| C114 | 0.57681 | 1.65035 | -0.8 |
| C115 | 0.60135 | 1.64629 | -0.89757 |
| C116 | 0.59249 | 1.58458 | -0.93349 |
| S117 | 0.58588 | 1.72945 | -0.75669 |
| N118 | 0.55476 | 1.03669 | -0.76827 |
| N119 | 0.94471 | 1.47512 | -0.61526 |
| C120 | 0.99029 | 1.44955 | -0.60946 |
| C121 | 0.49141 | 0.98973 | -0.722 |
| C122 | 1.04994 | 1.48079 | -0.66772 |
| C123 | 1.0968 | 1.45925 | -0.65873 |
| C124 | 1.08494 | 1.4066 | -0.59095 |
| C125 | 1.02597 | 1.37563 | -0.53173 |
| C126 | 0.97884 | 1.39688 | -0.54078 |
| C127 | 0.45191 | 0.92607 | -0.76769 |
| C128 | 0.38922 | 0.88008 | -0.72661 |
| C129 | 0.36549 | 0.89696 | -0.63823 |
| C130 | 0.40577 | 0.95886 | -0.58927 |
| C131 | 0.46902 | 1.00471 | -0.62995 |
| S132 | 0.28222 | 0.84002 | -0.58922 |
| O133 | 0.23791 | 0.7724 | -0.65648 |
| O134 | 0.23612 | 0.87466 | -0.5799 |
| O135 | 0.28103 | 0.81349 | -0.47291 |
| S136 | 1.14605 | 1.37945 | -0.57864 |
| O137 | 1.17684 | 1.39293 | -0.46855 |
| O138 | 1.113 | 1.30169 | -0.58522 |
| O139 | 1.21327 | 1.41094 | -0.66373 |
| O140 | 0.54731 | 1.75602 | -0.83119 |
| O141 | 0.55856 | 1.72957 | -0.64116 |
| O142 | 0.66212 | 1.79107 | -0.757 |
| H143 | 0.68181 | 1.12601 | -0.81468 |
| H144 | 0.734 | 1.24887 | -0.82551 |
| H145 | 0.54539 | 1.23358 | -0.7388 |
| H146 | 0.49219 | 1.11115 | -0.73935 |
| H147 | 0.7868 | 1.43615 | -0.86336 |
| H148 | 0.90101 | 1.49788 | -0.79313 |
| H149 | 0.83753 | 1.365 | -0.52945 |
| H150 | 0.7259 | 1.2991 | -0.60548 |

| | | | |
|---|---|---|---|
| H151 | 0.7048 | 1.45177 | -0.71047 |
| H152 | 0.64867 | 1.50982 | -0.762 |
| H153 | 0.52201 | 1.34377 | -0.97997 |
| H154 | 0.57613 | 1.28327 | -0.92628 |
| H155 | 0.50838 | 1.48612 | -0.72639 |
| H156 | 0.5229 | 1.59477 | -0.66441 |
| H157 | 0.62591 | 1.69043 | -0.94667 |
| H158 | 0.61018 | 1.58185 | -1.01023 |
| H159 | 0.57979 | 1.01593 | -0.80817 |
| H160 | 0.96673 | 1.52742 | -0.62488 |
| H161 | 1.06001 | 1.52174 | -0.72056 |
| H162 | 1.1425 | 1.48378 | -0.70403 |
| H163 | 1.01735 | 1.33604 | -0.47676 |
| H164 | 0.93523 | 1.37408 | -0.49084 |
| H165 | 0.46966 | 0.91257 | -0.83632 |
| H166 | 0.35884 | 0.83189 | -0.76419 |
| H167 | 0.38829 | 0.97162 | -0.51962 |
| H168 | 0.50002 | 1.05216 | -0.59038 |
| H169 | 1.2418 | 1.39289 | -0.63807 |

**Table S4** ICP-OES results of TfaTta-MB.

| Sample | $M_0$ (g) | $V_0$ (mL) | Test element | $C_0$ (mg/L) | $C_1$ (mg/L) | $C_x$ (mg/kg) | W (%) |
|---|---|---|---|---|---|---|---|
| TfaTta-MB | 0.0157 | 25 | S | 12.887 | 12.887 | 20520.70 | 2.05 |

**Table S5** Summary of the methods for sensing DMA and DCN.

| Analyte | Method | Linear range/μM | LOD/μM | Ref |
|---|---|---|---|---|
| DMA | competitive indirect enzyme-linked immunosorbent assay (CI-ELISA) | 0.045-45 | 0.01 | [S1] |
| | surfactant assisted electromembrane extraction (SEME) | 0.09–3.2 | 0.027 | [S2] |
| | Capillary electrophoresis-ultra violet (CE-UV) | 0.13–2.3 | 0.045 | [S3] |
| | lateral flow immunochromatographic strip (LFIC) | 0–1.4 | 0.45 | [S4] |
| | Fluorescence | 1–100 | 0.0241 | This method |
| DCN | Fluorescence | 0.3−30 | 0.12 | [S5] |
| | Fluorescence | 0.46−59.64 | 0.14 | [S6] |

| | | | | |
|---|---|---|---|---|
| | Fluorescence | 0-120 | 0.67 | [S7] |
| | Fluorescence | 0-100 | 0.95 | [S8] |
| | Fluorescence | 0-19 | 1.9 | [S9] |
| | Fluorescence | 5 – 1000 | 0.128 | This method |

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